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The Wiener-Hermite expansions of the Langevin transitions.

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Abstract

New partial differential equations for the Wiener-Hermite expansions of the Langevin (stochastic) transitions are formulated. They are solved recursively in full order series solutions with respect to \sqrt{t} . A sort of 'gauge' degrees of freedom (arbitrariness) involved in the solutions are analyzed and clarified. The Wiener-Hermite expansions play important roles as basic elements of numerical simulations of the Langevin equations. Specific solutions within some orders are presented as examples. These expansions giving integral representations of the Fokker-Planck evolution kernels, similar formulations are possible for the imaginary time Hamiltonian evolution kernels as well.

It is a long time since an idea that one expands stochastic variables of interest in terms of some normal ones, say, whose distributions are Gaussians, was emphasized by Wiener [1] as an important concept when discussing stochastic processes, e.g., diffusions. Diffusion processes with drift are modeled in the Langevin equations in use of idealized white noise terms as, $\dot{x}_i = u_i(x) + \eta_i(t)$ ($i = 1, 2, \dots, d$), with $\langle \eta_i(t) \eta_j(t') \rangle = 2\delta_{ij}\delta(t - t')$, and $\langle \eta_i(t) \rangle = 0$, where x_i denotes a position of a particle in d -dimensional flat space. These stochastic differential equations [2] define a transition, $X_i(t) = x_i(t) - x_{0i}$ for a finite time lapse t with an initial condition, $x_i(0) = x_{0i}$. It is a natural question to ask if one can obtain a suitable expansion of the Langevin

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transition $X_i(t)$ in terms of Gaussian random variates so that the expansion should have the same transition density as $X_i(t)$, i.e., a weak solution. One calls this the Wiener-Hermite expansion [3, 1, 4, 5]. The Langevin equations play important roles in wide range, from theoretical issues in physics such as stochastic quantization [6] together with its numerical applications in lattice field theories [9], to many applications in various fields of science and technology [7, 8]. These expansions have proper significance in numerical simulations of the Langevin equations since a finite number of Gaussian variates replace white noise, naively, a set of infinite number of Gaussian variates. Since explicitly solvable Langevin equations [7, 8] are restricted, approximations of solutions become important in practical applications. One can see in an extensive review [7] that quite a few approximation schemes have been examined in a long history of numerical applications of the Langevin equations, and yet the problem of systematic analysis of the approximation schemes is open. A reasonably systematic analysis toward higher order approximation schemes (weak Taylor approximation scheme [7]) was reported lately within any fixed finite order [10]. It is, however, welcome to obtain the Wiener-Hermite expansions of the Langevin transitions $X_i(t)$ in full order series solutions with respect to \sqrt{t} . Then these solutions will serve as basic elements for development of new schemes as Runge-Kutta like ones.

In this paper, we report a new successful formulation to obtain the Wiener-Hermite expansions in use of partial differential equations of $X_i(t)$ with respect to \sqrt{t} and d independent Gaussian random variates ξ_i with variance 2 and mean 0. They are solved recursively in full order series solutions with respect to \sqrt{t} . A sort of 'gauge' degrees of freedom (arbitrariness) can be involved in the solutions, and they are analyzed and clarified below.

Formulation and solutions in the flat space. One can derive from the Langevin equations (see, e.g., [6, 7, 8]) the corresponding Fokker-Planck equations $\partial_t P(t, x; 0, x_0) = K P(t, x; 0, x_0)$, for the transition density P , where $K = \partial_i(\partial_i - u_i(x))$, with an initial condition $P(0, x; 0, x_0) = \delta(x - x_0)$. Now the problem to solve is to find a vector function $X_i(t)$ whose variables are t and ξ_i , with parameters, values of u_i 's and their higher derivatives evaluated at x_0 , satisfying

$$e^{tK} \delta(x - x_0) = \langle \delta(x - x_0 - X(t)) \rangle, \quad (1)$$

where $\langle \dots \rangle$ is averaging over the Gaussian distribution of ξ_i . This equation (1) can be rewritten as a sort of integral representation of the Fokker-Planck evolution kernel as follows,

$$\langle x | e^{t\hat{K}} | x_0 \rangle = \langle x | \langle e^{-X \cdot \hat{\partial}} | x_0 \rangle , \quad (2)$$

where Dirac's notation is used, and it is to be noted that $\hat{K} = \hat{\partial}_i(\hat{\partial}_i - u_i(\hat{x}))$ and that the evolution operator on the l.h.s. is arranged in normal order (all $\hat{\partial}$'s in left of all \hat{x} 's). By differentiating (2) with respect to t , to obtain $\langle (K + \partial_t X \cdot \partial_x) e^{-X \cdot \partial_x} \rangle \langle x | x_0 \rangle = 0$, and then replacing the argument x of u_i in K with $x_0 + X$, and dropping off $\langle x | x_0 \rangle$, one derives an operator equation as,

$$\langle (\partial_x^2 - u \cdot \partial_x + \partial_t X \cdot \partial_x) e^{-X \cdot \partial_x} \rangle = 0 , \quad (3)$$

where one may consider either that only differential operators ∂_x are involved with all the other parameters or that all operators are normal-ordered. Putting $X_i = s\xi'_i$, where $s = \sqrt{t}$, one assumes that the unknown ξ'_i is to be expanded as $\xi'_i = \xi_i + \text{higher orders w.r.t. } s$, as a standard choice [7, 11]. It implies that ξ' and ξ can be expanded perturbatively with each other, and that the unknown is the coordinate transformation between them. Replacing ∂_x in (3) with $-(1/s)D'$, where and hereafter D' and D denote $\partial_{\xi'}$ and ∂_{ξ} , respectively, and noting $\langle \dots \rangle = \text{const} \times \int d\xi e^{-\frac{1}{4}\xi^2} \dots$, and making use of the partial integration formula and of change of integration variables to ξ' to have a form of the Fourier transformation, one obtains after some calculation on (3) the following partial differential equation as,

$$D_k \left[e^{-\frac{1}{4}\xi^2} \left(\frac{1}{D\xi'} \right)_{ik} \left\{ \frac{\partial X_i}{\partial t} - \frac{1}{2s}(\xi_j - 2D_j) \left(\frac{1}{D\xi'} \right)_{ij} - u_i(x_0 + s\xi') \right\} \right] = 0 , \quad (4)$$

where matrix notation is used, e.g., $(D\xi')_{ij} = \partial_{\xi_i} \xi'_j$, and summation over repeated indices should be understood. If one puts $\xi'_i = \xi_i + sy_i$, then one can derive from (4) the following partial differential equation as,

$$D_k \left[e^{-\frac{1}{4}\xi^2} \left(\frac{1}{D\xi'} \right)_{ik} \left\{ (1 + s\partial_s + M)_{ij} y_j - s(\xi_j - 2D_j) \left(\frac{1}{1 + sDy} (Dy)^2 \right)_{ij} - 2u_i(x_0 + s\xi') \right\} \right] = 0 , \quad (5)$$

where an operator M_{ij} is defined as $M_{ij} = D_i(\xi_j - 2D_j)$. Since we assume series solutions of y_i with respect to s , and assume that each order

is given by a polynomial of ξ_i , we define a space F of vector functions as $F = \{f_i = p_i e^{-\frac{1}{4}\xi^2} \mid p_i \text{ is a polynomial of } \xi\}$. A basis of this space can be spanned by those functions f_i 's as, $f_i = C_{i,i_1,i_2,\dots,i_n} D_{i_1} D_{i_2} \cdots D_{i_n} e^{-\frac{1}{4}\xi^2}$, where the polynomial part is essentially the generalized Hermite polynomial. It is to be noted that any coefficient tensor C_{i,i_1,i_2,\dots,i_n} can be decomposed uniquely into totally symmetric component with respect to all indices including i and the residual component. The decomposition of coefficient tensors defines decomposition of F . We denote a space of the totally symmetric component as F_S , and a space of the residual component as F_{PNS} , and $F = F_S + F_{PNS}$. Here we name $f_i \in F_S$ as a *symmetric vector function*, and $f_i \in F_{PNS}$ as a *pure nonsymmetric vector function*. Then for $f_i \in F$, $D_i f_i = 0$ implies f_i is a pure nonsymmetric vector function. A space P of polynomial vector function p_i can be defined as $P = \{p_i \mid p_i = e^{\frac{1}{4}\xi^2} f_i, f_i \in F\}$, and $P = P_S + P_{PNS}$ with similarly defined P_S and P_{PNS} , where P_S is a space of *symmetric vector polynomials* and P_{PNS} *pure nonsymmetric vector polynomials*. One sees for $p_i \in P_{PNS}$, that $M_{ij} p_j = 0$, and can show for $p_i \in P_S$, in a form as $p_i = e^{\frac{1}{4}\xi^2} C_{i,i_1,i_2,\dots,i_n} D_{i_1} D_{i_2} \cdots D_{i_n} e^{-\frac{1}{4}\xi^2}$, that $M_{ij} p_j = (n+1)p_i$ [12]. Thus it is clear how P splits into eigenspaces of M . Now one can derive the following equation from (5) in use of an arbitrary $a_i \in P_{PNS}$, as,

$$\begin{aligned} \left\{ (1 + s\partial_s + M)(y - u - a) \right\}_i &= s(\xi_j - 2D_j) \left(\frac{1}{1 + sD_y} (Dy)^2 \right)_{ij} \\ &\quad + 2(e^{(s\xi + s^2 y) \cdot \partial_x} - 1)u_i + s((1 + s\partial_s)a_j)(Dy)_{ji} \quad (6) \end{aligned}$$

where the Taylor expansion of $u_i(x_0 + s\xi')$ at x_0 should be understood. Since eigenvalues of the operator $1 + s\partial_s + M$ are positive in view of our assumption for solutions y_i , one easily obtains the following recursion formula for a series solution $y_i = \sum_{n=0}^{\infty} s^n y_{i(n)}$, for $n > 0$ as

$$\begin{aligned} y_{i(n)} &= a_{i(n)} + \frac{1}{1 + n + M} \left\{ (\xi_j - 2D_j) \left(\frac{1}{1 + sDY} (DY)^2 \right)_{ij} \right. \\ &\quad \left. + \frac{2}{s} (e^{(s\xi + s^2 Y) \cdot \partial_x} - 1)u_i + ((1 + s\partial_s)A)_j (DY)_{ji} \right\}_{(n-1)} \quad (7) \end{aligned}$$

where $A_i = \sum_{k=0}^{n-1} s^k a_{i(k)}$, and $Y_i = \sum_{k=0}^{n-1} s^k y_{i(k)}$, and $\{\cdots\}_{(m)}$ denotes m -th order terms of $\{\cdots\}$, and for $n = 0$, $y_{i(0)} = u_i + a_{i(0)}$. The partial differential equation (4) and the recursion formula (7) for its series solution are main results of the present work. One notes that arbitrariness of the solution, a

sort of 'gauge' degrees of freedom, comes from $a_i \in P_{PNS}$, and it is interesting to note that $a_i e^{-\frac{1}{4}\xi^2}$ appears as a transverse vector function in a space of d -dimensional Gaussian random variates. Actual calculation of $1/(1+n+M) \cdot \{\dots\}$ in (7) is easy in principle, and it is readily done if decomposition of $\{\dots\}$ in eigenfunctions of M is obtained. Let p_i be a given k -th order polynomial of ξ . Then p_i is written as a linear combination of $k+2$ unknown eigenfunctions. By multiple operations of M on the equation, one obtains sufficient number of independent equations to solve the unknowns.

Example of $O(s^6)$ expansion of X_i in the flat space. Specific example of the solution X_i given by (7) can be chosen arbitrarily to some extent as stated above. We give an example in simplicity principle as follows,

$$\begin{aligned} X_i(s, \xi, x_0) = & s\xi_i + s^2 u_i + \frac{s^3}{2} \xi_j \partial_j u_i + \frac{s^4}{6} (\xi_j \xi_k \partial_j \partial_k u_i + 3u_j \partial_j u_i + \partial^2 u_i) \\ & + \frac{s^5}{24} (8\xi_j u_k \partial_j \partial_k u_i + 4\xi_j \partial_j u_k \partial_k u_i + \xi_j \partial_k u_j \partial_k u_i + \xi_j \xi_k \xi_m \partial_j \partial_k \partial_m u_i + 2\xi_j \partial_j \partial^2 u_i) \\ & + \frac{s^6}{6} (2\partial_j u_k \partial_j \partial_k u_i + u_j u_k \partial_j \partial_k u_i + \partial^2 u_j \partial_j u_i + u_j \partial_j u_k \partial_k u_i + 2u_j \partial_j \partial^2 u_i + \partial^2 \partial^2 u_i) \quad (8) \end{aligned}$$

where, for brevity's sake, those eigenfunctions with eigenvalues other than $M = 1$ are dropped off in $O(s^6)$, which only affect higher orders in calculation of expectation values of any quantities. In the process of the above derivation, a_i is so chosen as to cancel out $\partial_j u_j$ from the expression. The result (8) coincides with the former result obtained in a different approach [10], except for allowable deviation of $M = 4$ eigenfunction in $O(s^5)$ terms for the same reason as in $O(s^6)$. We give a brief interpretation on that arbitrariness encountered here other than those in the full order expansion of X_i , which is characteristic to the finite order approximation. Suppose that one obtains the full order series solution X_i and one is to use it in the transition density (1) within some finite order, say $O(s^6)$. It is needless to say that one only has to retain terms in X_i up to $O(s^6)$, and it is only required to give correct expectation values of all moments of X_i within $O(s^6)$. Let us consider, for example, roles of $O(s^5)$ terms in calculation of $\langle (X_i)^m \rangle$, and we note that only relevant cases are when $m = 1, 2$, since the leading order of X_i is $O(s)$ and that $\langle O(s^5) \text{ terms} \rangle = 0$ if $m = 1$. When $m = 2$, only $\langle s\xi \cdot (O(s^5) \text{ terms}) \rangle$ is important. Key observation is that $\langle (\xi)^k \cdot (M = n) \text{ eigenfunction} \rangle = 0$

if $k < n - 1$. Thus ($M = n$) *eigenfunction* with $n = 4, 6, \dots$ may be subtracted in $O(s^5)$ terms in X_i within the $O(s^6)$ approximation scheme. In the previous work [10], actual performance of the present $O(s^6)$ algorithm in numerical simulation of Langevin equation was tested in application to a single degree of freedom $U(1)$ statistical model, where a significant improvement over $O(s^4)$ algorithm was observed in data in a theoretically expected manner.

Formulation and solutions in the Lie group space. The present method for the Wiener-Hermite expansion can be extended to the Langevin transition in the Lie group space. We give a brief interpretation on the formulation and its solutions. Specifically we assume the Lie group is $SU(N)$. The Langevin equation in the case [13, 14] reads as $g^{-1} \frac{d}{dt} g = \lambda_i(u_i + \eta_i)$ where $g \in SU(N)$ and λ_i 's ($i = 1, \dots, N^2 - 1$) form antihermitean basis of Lie algebra, $[\lambda_i, \lambda_j] = c_{ijk} \lambda_k$ with normalization $\text{tr}(\lambda_i^\dagger \lambda_j) = \delta_{ij}$, and η_i 's are white noises as given above. The corresponding Fokker-Planck equation reads as $\partial_t \phi = K \phi$, where ϕ is normalized as $\int d\mu \phi = 1$ with the Haar measure $d\mu$, and $K = \nabla_i(\nabla_i - u_i)$, and ∇_i 's are right differentiations as defined in $e^{\epsilon \cdot \nabla} f(g) = f(g e^{\epsilon \cdot \lambda})$ for any functions f on $SU(N)$, and it holds $[\nabla_i, \nabla_j] = c_{ijk} \nabla_k$. Definition of the transition X_i is given as $e^{tK} \delta^{inv}(g - g_0) = \langle e^{-X \cdot \nabla} \delta^{inv}(g - g_0) \rangle$, where δ^{inv} is an *invariant* δ -function, and it holds $\delta^{inv}(g e^{-X \cdot \lambda} - g_0) = \delta^{inv}(g - g_0 e^{X \cdot \lambda})$. Line of reasoning to reach a partial differential equation for X_i is parallel to that of (4) except for non-commutativity of differentiation ∇_i 's. We make use of left differentiation \mathcal{D}_i with respect to $e^{x \cdot \nabla}$ such that $\mathcal{D}_i e^{x \cdot \nabla} = \nabla_i e^{x \cdot \nabla}$, where $-\mathcal{D}_i$'s satisfy the same commutation relations as λ_i 's and can be written as $\mathcal{D}_i = (h(x \cdot C))_{ij} \partial_{x_j}$ with a function h of a single variable x , $h(x) = (-x)/(e^{-x} - 1)$, and with matrices $(C_i)_{jk} = c_{ikj}$, ($i = 1, \dots, N^2 - 1$). The corresponding equation to (4) reads as follows,

$$D_k \left[e^{-\frac{1}{4} \xi^2} \left(\frac{1}{D \xi'} \right)_{ik} \left\{ \frac{\partial X_i}{\partial t} - \frac{1}{2s} h_{im}^t (\xi_j - 2D_j) \left(h \frac{1}{D \xi'} \right)_{mj} - h_{im}^t u_m (g_0 e^{s \xi' \cdot \lambda}) \right\} \right] = 0, \quad (9)$$

where $h_{ij} = (h(-X \cdot C))_{ij}$ and $X_i = s\xi'_i$. To (5) corresponds the following equation as,

$$D_k \left[e^{-\frac{1}{4}\xi^2} \left(\frac{1}{D\xi'} \right)_{ik} \left\{ (1 + s\partial_s + M)_{ij} y_j - s \left(h^t L_j h \frac{1}{1 + sDy} (Dy)^2 \right)_{ij} - 2h_{im}^t u_m (g_0 e^{s\xi'}) - \frac{1}{s} \left((h^t L_j h - L_j)(1 - sDy) \right)_{ij} \right\} \right] = 0, \quad (10)$$

where $L_j = \xi_j - 2D_j$ and $h = 1 + sw$ are operators, and $w = w(sy, \xi, s)$. Now it is derived in the same way as before in use of an arbitrary $a_i \in P_{PNS}$ that

$$\begin{aligned} \left\{ (1 + s\partial_s + M)(y - u - a) \right\}_i &= s \left(h^t L_j h \frac{1}{1 + sDy} (Dy)^2 \right)_{ij} \\ &\quad + 2(h^t e^{(s\xi + s^2 y) \cdot \nabla} - 1)_{ik} u_k + (h^t L_j w)_{ij} + w_{ij}^t \xi_j \\ &\quad - s \left((w^t L_j + L_j w + s w^t L_j w)(DY) \right)_{ij} + s((1 + s\partial_s) a_j)(DY)_{ji}. \end{aligned} \quad (11)$$

The recursion formula for a series solution $y_i = \sum_{n=0}^{\infty} s^n y_{i(n)}$, for $n > 0$ reads as

$$\begin{aligned} y_{i(n)} &= a_{i(n)} + \frac{1}{1 + n + M} \left\{ s \left(H^t L_j H \frac{1}{1 + sDY} (DY)^2 \right)_{ij} \right. \\ &\quad + 2(H^t e^{(s\xi + s^2 Y) \cdot \nabla} - 1)_{ik} u_k + (H^t L_j W)_{ij} + W_{ij}^t \xi_j \\ &\quad \left. - s \left((W^t L_j + L_j W + s W^t L_j W)(DY) \right)_{ij} + s((1 + s\partial_s) A_j)(DY)_{ji} \right\}_{(n)}, \end{aligned} \quad (12)$$

where $Y_i = \sum_{k=0}^{n-1} s^k y_{i(k)}$, $A_i = \sum_{k=0}^{n-1} s^k a_{i(k)}$, $W = w(sY, \xi, s)$, and $H = 1 + sW$ on the right hand side, and for $n = 0$, $y_{i(0)} = u_i + a_{i(0)}$.

Example of $O(s^4)$ expansion of X_i in the Lie group space. Specific example of the solution X_i due to (12) can be given as follows,

$$X_i(s, \xi, g_0) = s\xi_i + s^2 u_i + \frac{s^3}{2} \left(\xi_j \nabla_j u_i - \frac{N}{6} \xi_i \right) + \frac{s^4}{6} (3\nabla^2 u_i + 3u_j \nabla_j u_i + N u_i), \quad (13)$$

where for brevity's sake, only $M = 1$ eigenfunction is retained in $O(s^4)$ for the reason characteristic to finite order approximation as stated above, and $u_i = \nabla_i S$ is used. The result (13) shows that (12) reproduces correctly the one previously obtained [13].

Discussions and outlooks Some remarks are in order with respect to the Wiener-Hermite expansion of the Langevin transition X_i in the present formulation. First of all, in view of (1) and (2), it is obviously useful in numerical simulation of distribution $\langle x|e^{TK}|x_0\rangle$ with a fixed x_0 , and $T = nt$, where a choice of n sets of d independent Gaussian random varieties, i.e., those in nd dimensions, determines a discrete path, and an $O(t^{k+1})$ approximation of X_i yields $O(1/n^k)$ one for the distribution for the time T [13, 7]. Another point to remark is that one obtains a distribution function $\langle x|e^{TK}|x_0\rangle$ of x by finding an inverse function $\xi = \xi(\xi')$ of $\xi'(\xi)$ and by substituting $\xi' = (x - x_0)/s$ to $const \cdot \det(\frac{\partial \xi}{\partial \xi'}) e^{-\frac{1}{4}\xi^2}$. A counterpart in the Lie group space of this observation holds as well, if one defines properly a distribution function ψ in noncompact space of the canonical coordinate of the first kind, X , with $g = g_0 e^{X \cdot \lambda}$ so that $\int dX \psi(X) f(g) = \int d\mu(g) \langle g|e^{tK}|g_0\rangle f(g)$, and then it is given as $\psi = const \cdot \det(\frac{\partial \xi}{\partial \xi'}) e^{-\frac{1}{4}\xi^2}|_{\xi'=X/s}$. In view of the defining equation (2) of the Wiener-Hermite expansion X_i , one can see obvious extensions of the present formulation to cases where on the left hand side of (2) the Fokker-Planck evolution operators are arranged in other orderings, e.g., the Weyl ordering, instead of the normal one. Then one can have the X_i depending on both parameters x_0 and x , which is so called implicit algorithms in [7]. Another extension of the present formulation is toward the case where the imaginary time Hamiltonian evolution operators e^{-tH} are treated in various operator orderings. Then we need an extra scalar function in the exponent of the right hand side of (2), since the distribution is not normalized any more. This extension will also give means of numerical simulations of the ground state in such systems of interest provided shrinking of the distribution is properly taken care of. Finally we comment that a ξ -linear solution is correctly reproduced from (7) with $a_i = 0$ for the Ornstein-Uhlenbeck process [8], the case u_i being linear functions. We conclude that main results of the present work are the partial differential equations (4) and (9) together with their solutions (7) and (12), respectively, and that although their mathematical rigorousness on a level of [2, 7] such as convergence of the series solutions is beyond scope of the present analyses, we believe those will play important roles as a basis for systematic development of weak approximation schemes including Runge Kutta like ones.

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